

# Aiding the Convergence of Numerical Integration in the presence of Singularities

Charles Kankelborg

January 17, 2020

Non-analytic features such as singularities can, in principle, be integrated with any open scheme such as the midpoint Romberg methods.<sup>1</sup> However, convergence tends to be very slow. For singularities, the error in the result typically falls off more slowly than  $1/N$ , and the rate is almost independent of the order of the quadrature. Let us write such a definite integral this way:

$$I = \int_0^d f(x) dx. \quad (1)$$

Without loss of generality, I have assumed that the non-analytic point occurs at  $x = 0$ . If it is a singularity, then  $f(x)/a \rightarrow \infty$  as  $x \downarrow 0$ . Suppose we expand the integrand in the following fashion:

$$f(x) = \frac{a + bx + \mathcal{O}(x^2)}{x^\gamma}, \quad 0 < \gamma < 1. \quad (2)$$

If  $a \neq 0$ , then there is an integrable singularity at  $x = 0$ . If  $a = 0$  but  $b \neq 0$ , then there is a singularity in the derivatives of the integrand. For small  $x$ , the integrand may be approximated as

$$f(x) \approx h(x) = ax^{-\gamma} + bx^{1-\gamma}. \quad (3)$$

This expression may be integrated analytically. Using the trivial substitution  $f = f - h + h$ , the integral may therefore be rewritten

$$I = \int_0^d [f(x) - ax^{-\gamma} - bx^{1-\gamma}] dx + \frac{ad^{1-\gamma}}{1-\gamma} + \frac{bd^{2-\gamma}}{2-\gamma}. \quad (4)$$

---

<sup>1</sup>See, e.g., Press et al., *Numerical Recipes in C*.

The new integrand in the above expression is superior to  $f(x)$  for numerical purposes, because it is well behaved at  $x = 0$ , and so the quadrature with a high order method will usually converge rapidly. The terms outside the integral may be evaluated trivially.

If both  $a$  and  $b$  are nonzero but we ignore the  $b$  term in “fixing up” the integral, then we will find that the convergence is only a little improved, usually to between  $1/N$  and  $1/N^2$ .

If there is also a non-analytic feature at  $d$ , it can be corrected in the same manner after a change of variable to place  $d$  at the origin. If there are singularities in the interior, the integral can be broken up to deal with each one in turn.